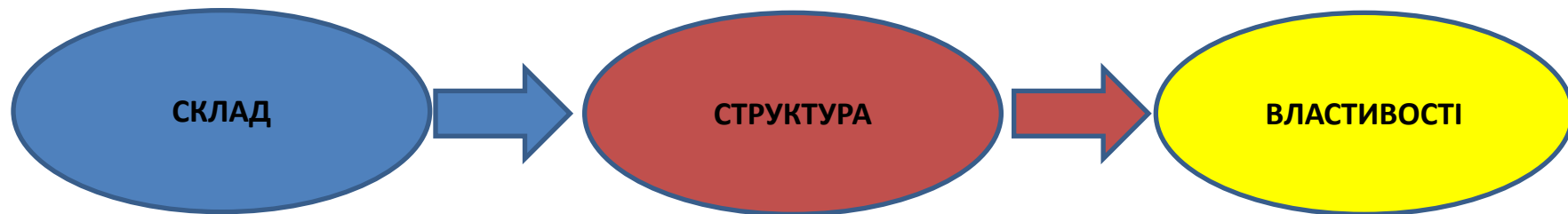# Комп'ютерне моделювання електронних властивостей матеріалів

Лабораторна робота 1
Вступ до Quantum Espresso

Олег Фея, к.ф-м.н

КОМП'ЮТЕРНИЙ ДИЗАЙН МАТЕРІАЛІВ

СКЛАД → СТРУКТУРА → ВЛАСТИВОСТІ

ДОСЛІДНИЦЬКІ МЕТОДИ

Експеримент

Розрахунки: теорія функціоналу густини (FPLO, VASP, Abinit, Wien2k),
Еволюційні алгоритми (USPEX, CALLYPSO...)...

Quantum Espresso

The Quantum ESPRESSO community stands by the Ukrainian people and expresses its concerns for the devastating effects that the Russian military offensive has on their country and on the free and peaceful scientific, cultural, and economic cooperation amongst peoples.

QUANTUMESPRESSO

Quantum Espresso

QUANTUM ESPRESSO is an open initiative, in collaboration with many groups world-wide, coordinated by the QUANTUM ESPRESSO Foundation. Present members of the latter include Scuola Internazionale Superiore di Studi Avanzati (SISSA) , the Abdus Salam International Centre for Theoretical Physics (ICTP), the CINECA National Supercomputing Center, the Ecole Polytechnique Fédérale de Lausanne, the Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin. Courses on modern electronic-structure theory with hands-on tutorials on the QUANTUM ESPRESSO codes are offered on a regular basis in collaboration with ICTP.
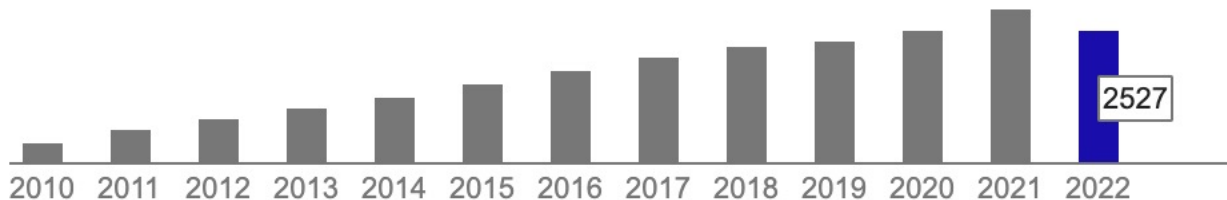
Quantum Espresso

Пласкі хвилі
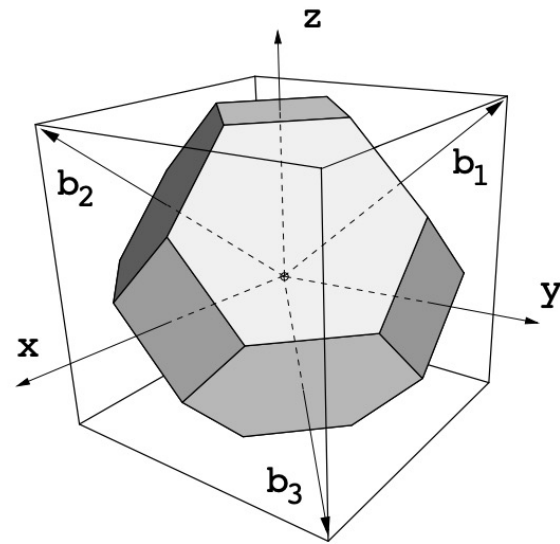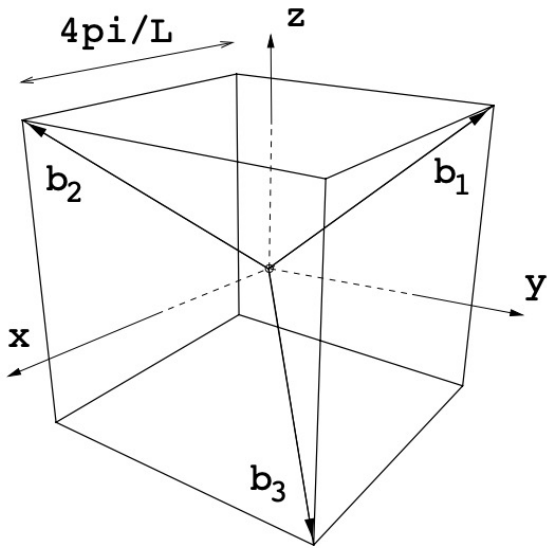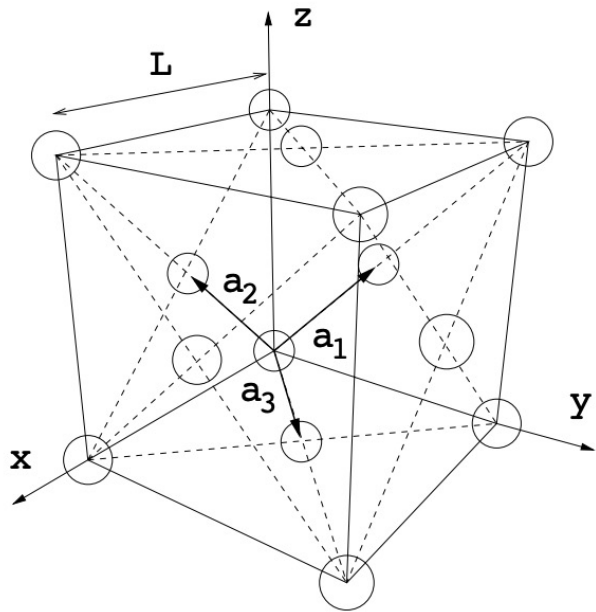
$$\psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})e^{i\mathbf{kr}}$$

$$u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

Обернений простір

$$\mathbf{b}_1 = \frac{2\pi}{\Omega}\mathbf{a}_2 \times \mathbf{a}_3 \quad \mathbf{b}_2 = \frac{2\pi}{\Omega}\mathbf{a}_3 \times \mathbf{a}_1 \quad \mathbf{b}_3 = \frac{2\pi}{\Omega}\mathbf{a}_1 \times \mathbf{a}_2$$
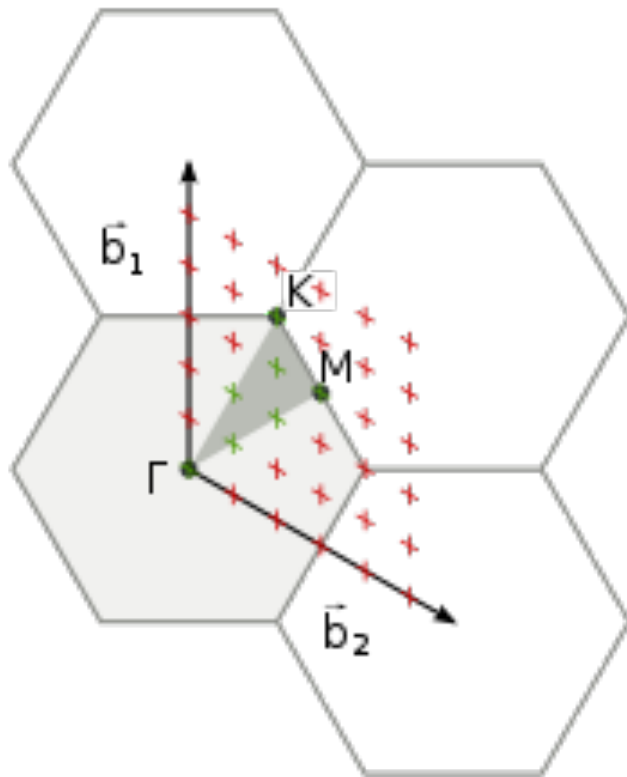
$$\Omega = \mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3 \qquad \mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$

Обернений простір

$$\rho(\mathbf{r}) = \frac{1}{\Omega_{\text{BZ}}} \sum_n \int_{\text{BZ}} f_{n\mathbf{k}} |\psi_{n\mathbf{k}}(\mathbf{r})|^2 d\mathbf{k}$$

$$\rho(\mathbf{r}) = \sum_{n\mathbf{k}} w_{\mathbf{k}} f_{n\mathbf{k}} |\psi_{n\mathbf{k}}(\mathbf{r})|^2 d\mathbf{k}$$

$$\frac{1}{2} |\mathbf{G} + \mathbf{k}|^2 < E_{\text{cutoff}}$$

Приклад вхідного файла

```
&control
   calculation = 'scf'
   prefix='silicon',
   pseudo_dir = './',
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
/
&electrons
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
/
ATOMIC_SPECIES
 Si  28.086  Si.pz-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS {automatic}
8 8 8 0 0 0
```
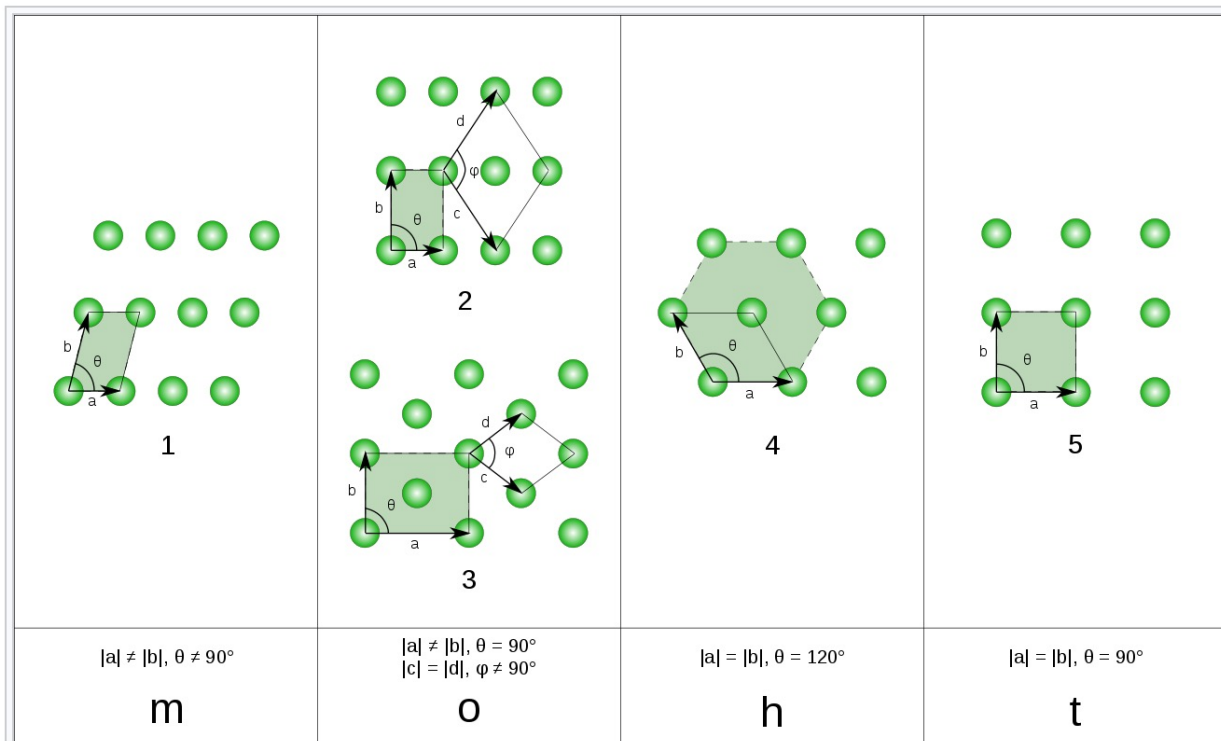
Приклад вхідного файла

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ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS {automatic}
8 8 8 0 0 0
```


$|a| \neq |b|$, $\theta \neq 90°$	$|a| \neq |b|$, $\theta = 90°$ $|c| = |d|$, $\varphi \neq 90°$	$|a| = |b|$, $\theta = 120°$	$|a| = |b|$, $\theta = 90°$
m	o	h	t

Приклад вхідного файла

```
&control
   calculation = 'scf'
   prefix='silicon',
   pseudo_dir = './',
 /
 &system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
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 /
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 /
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 Si  28.086  Si.pz-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS {automatic}
8 8 8 0 0 0
```
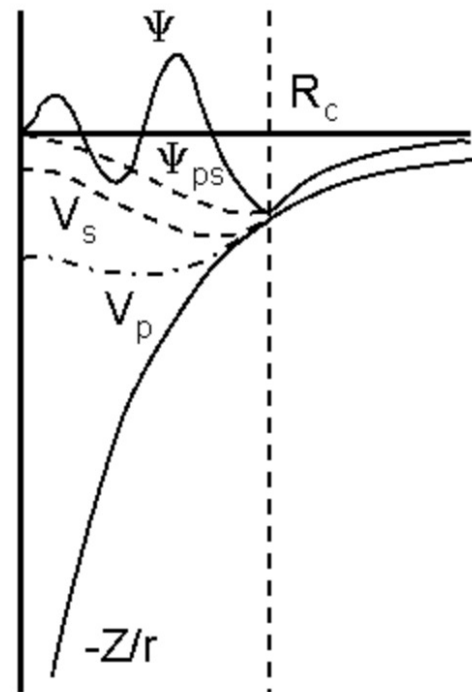
$$\frac{1}{2}|\mathbf{G} + \mathbf{k}|^2 < E_{\mathrm{cutoff}}$$

Приклад вхідного файла

```
&control
  calculation = 'scf'
  prefix='silicon',
  pseudo_dir = './',
/
&system
  ibrav= 2,
  celldm(1) =10.20,
  nat= 2,
  ntyp= 1,
  ecutwfc =18.0,
/
&electrons
  mixing_mode = 'plain'
  mixing_beta = 0.7
  conv_thr =  1.0d-8
/
ATOMIC_SPECIES
 Si  28.086  Si.pz-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS {automatic}
8 8 8 0 0 0
```
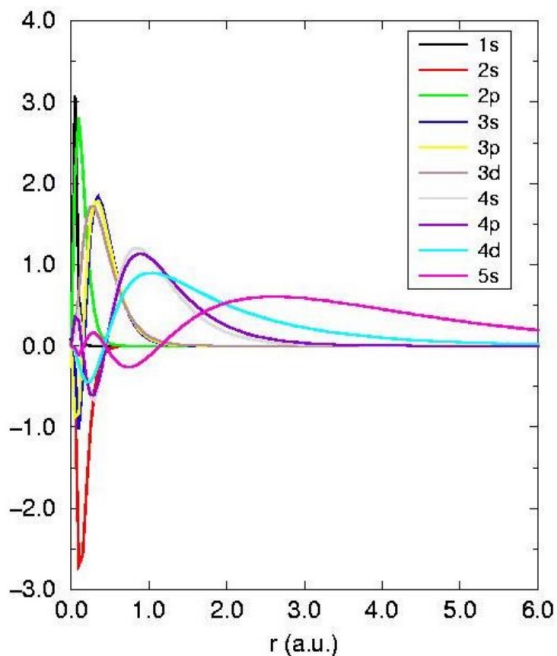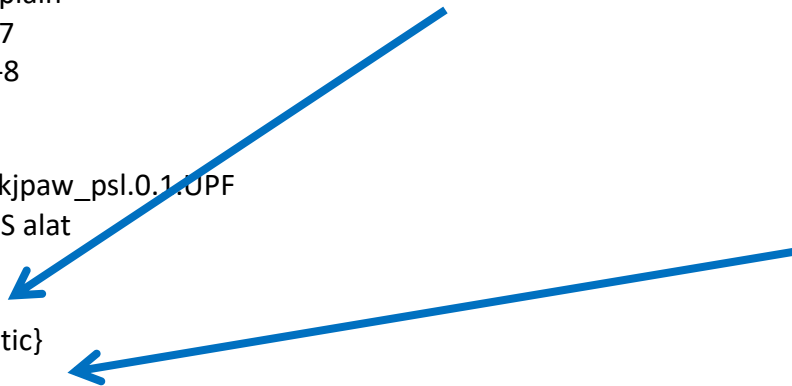
$[Kr]$, $4d^{10}$, $5s^1$, $5p^0$, $5d^0$

$\phi(r)$

Приклад вхідного файла

```
&control
   calculation = 'scf'
   prefix='silicon',
   pseudo_dir = './',
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
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ATOMIC_SPECIES
 Si  28.086  Si.pz-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS {automatic}
8 8 8 0 0 0
```
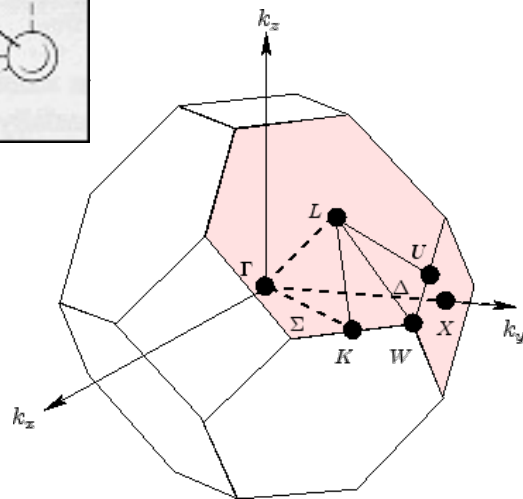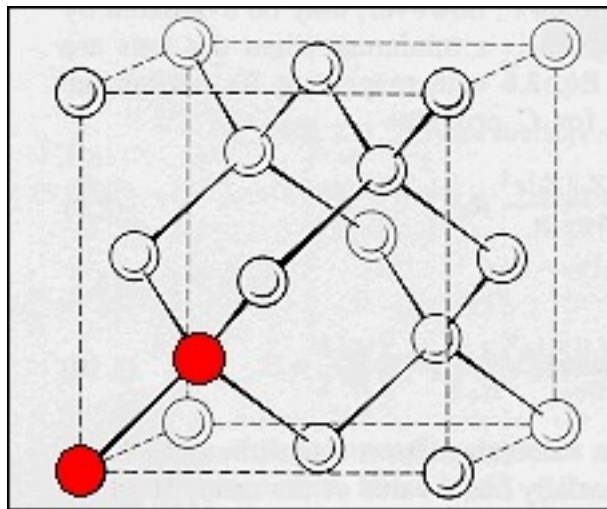
Приклад вхідного файла

```
&control
   calculation = 'scf'
   prefix='silicon',
   pseudo_dir = './',
   wf_collect=.true.
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
/
&electrons
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
/
ATOMIC_SPECIES
 Si  28.086  Si.pz-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS {automatic}
 8 8 8 0 0 0
```